Example 2b

June 17, 2020

1 Example 1b: Double well potential - Analyzing experimental data with pretrained network

Example code to analyze experimental data with DeepCalib using a pretrained network.

DeepCalib 1.0 Enhanced force-field calibration via machine learning version 1.0 - 27 April 2020 l' Aykut Argun, Tobias Thalheim, Stefano Bo, Frank Cichos & Giovanni Volpe Soft Matter Lab

1.1 1. INIZIALIZATION

```
In [1]: import DeepCalib
```

1.2 2. Import and visualize the experimental trajectory to be analyzed

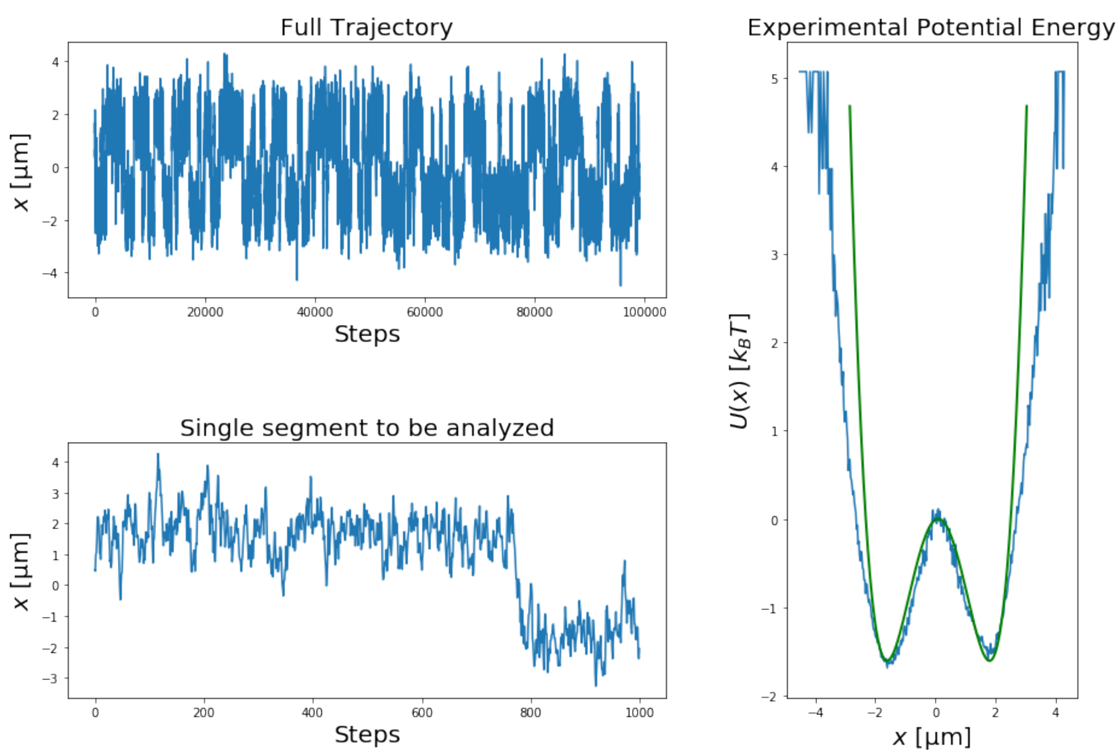
Here we import and visualize the experimental trajectory.

Comments: 1. Make sure you define the same scaling functions for the inputs and the targets the same in the training file.

```
In [2]: ### Import the data

        import scipy.io as sci
        data_name = 'Data_Example2b'
        x = sci.loadmat(data_name)['x']
        x = x[1];

        ### Visualize the trajectory

        import matplotlib.pyplot as plt
        %matplotlib inline
        fig = plt.figure(figsize=(15, 10))
        gs = fig.add_gridspec(10,10)
        plt.subplot(gs[0:4,0:6])
        plt.ylabel('$x$ [\u03BCm]',fontsize=20)
        plt.xlabel('Steps',fontsize=20)
        plt.title('Full Trajectory',fontsize=20)
        plt.plot(x)

        ### Visualize a single input for analysis
```

```
plt.subplot(gs[6:10,0:6])
plt.ylabel('$x$ [\u03BCm]',fontsize=20)
plt.xlabel('Steps',fontsize=20)
plt.title('Single segment to be analyzed',fontsize=20)
plt.plot(x[23000:28000:5])

### Visualize the measured truths

import numpy as np
l = (np.arange(400) - 200) * 0.025
h = np.histogram(x, bins = l)[0]
U = -np.log(h[h>0]) + np.log(h[round(h.size/2)])
plt.subplot(gs[:,7:10])
plt.xlabel('$x$ [\u03BCm]',fontsize=20)
plt.ylabel('$U(x)$ [$k_BT$]',fontsize=20)
plt.title('Experimental Potential Energy',fontsize=20)
plt.plot(l[np.append(h>0,False)],U)
L = 1.71
DU = 1.61
UH = DU*((l/L)**2-1)**2-DU
plt.plot(l[UH<5]+.1,UH[UH<5],c='green',Linewidth = 2)
```

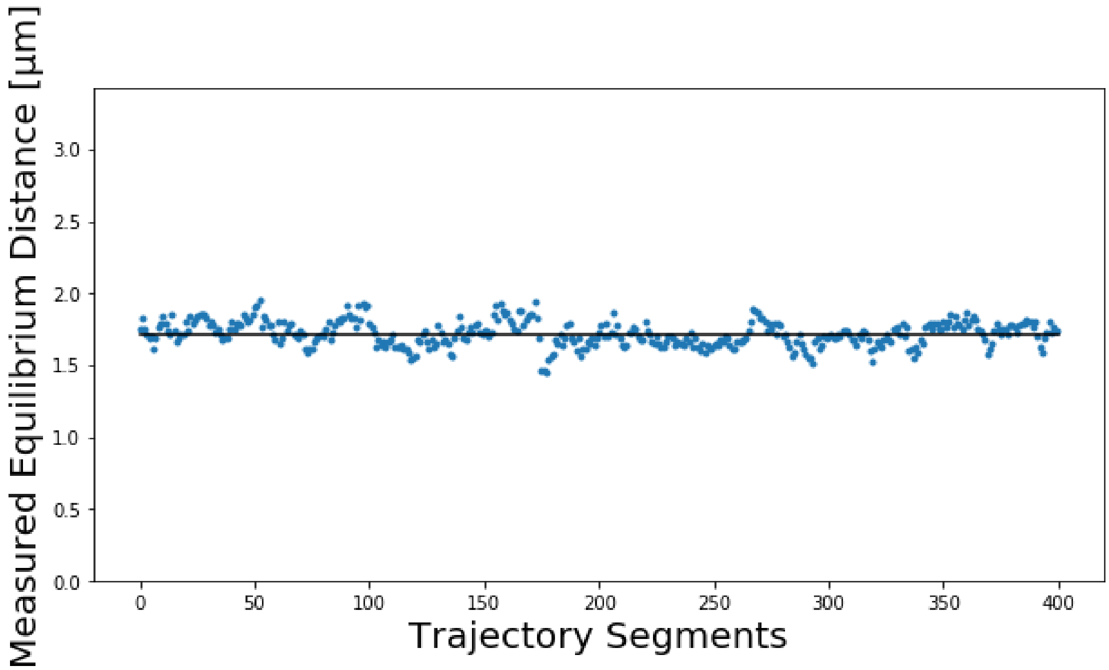
Out[2]: [<matplotlib.lines.Line2D at 0x221a9716390>]

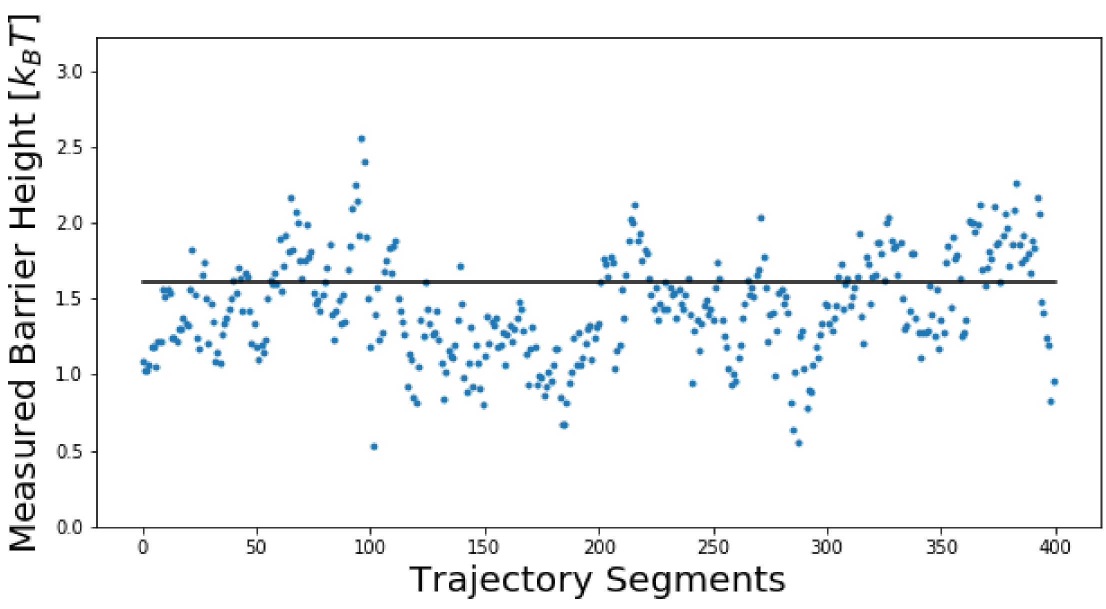


In [4]:
```
### Analyze the data

from keras.models import load_model
import numpy as np
from scipy.constants import Boltzmann as kB
network = load_model('Network_Example_2a.h5')
predictions_L = []
predictions_H = []
oversamp = 5
nmeas = 400
steps = int((x.size-1000*oversamp)/nmeas)
slength = 1000*oversamp
for i in range(nmeas):
    x_crop = x[(i*steps):(i*steps+slength):oversamp]
    predicted_L, predicted_H = DeepCalib.predict(network, x_crop)[0]
    predictions_L.append(predicted_L)
    predictions_H.append(predicted_H)

L0 = 2e-6
H0 = kB*300
rescale_targets = lambda scaled_L, scaled_H: [(1 + scaled_L)*L0,
                                              np.exp(scaled_H) * H0] # Inverse of target
[predictions_L, predictions_H] = rescale_targets(*np.array([predictions_L, predictions_H
```

In [5]:
```
fig = plt.figure(figsize=(10, 5))
plt.plot(predictions_L*1e6,'.')
plt.plot([0, 400], [L, L],color='black')
plt.ylim([0, 2*L])
plt.xlabel('Trajectory Segments',fontsize=20)
plt.ylabel('Measured Equilibrium Distance [\u03BCm]',fontsize=20)

fig = plt.figure(figsize=(10, 5))
plt.plot(predictions_H/kB/300,'.')
plt.plot([0, 400], [DU, DU],color='black')
plt.xlabel('Trajectory Segments',fontsize=20)
plt.ylim([0, 2*DU])
plt.ylabel('Measured Barrier Height [$k_BT$]',fontsize=20)
```

Out[5]:
```
Text(0, 0.5, 'Measured Barrier Height [$k_BT$]')
```


Measured Equilibrium Distance [µm]
0.0
0.5
1.0
1.5
2.0
2.5
3.0
0
50
100
150
200
250
300
350
400
Trajectory Segments


Measured Barrier Height [$k_B T$]
0.0
0.5
1.0
1.5
2.0
2.5
3.0
0
50
100
150
200
250
300
350
400
Trajectory Segments